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Lattice Boltzman Method for turbulent combustion

Sharath S. Girimaji, Texas A & M University
Li-Shi Luo, ICASE, NASA Langley Research Center

1 Introduction

Over the last few years, the Lattice Boltzman methods – Lattice Boltzman Equation (LBE) and Lattice Gas Automata (LGA) – have made significant strides in both theory and application On the theoretical front, rigorous mathematical proof now exists demonstrating that the LBE method is a special finite difference scheme of the *Boltzmann equation that governs all fluid flow* [1]. (Recall that the Navier-Stokes equation also has its basis in the Boltzmann equation.) It has also been shown that the LBE method can be related to some conventional CFD methods and the proof brings to light the advantages of the LBE method. Detailed numerical studies with the LBE method have demonstrated the physical accuracy and computational tractability for solving complex fluid flow problems. In its current state, the LBE method is fully developed and well-tested for moderate-Reynolds number, isothermal flows. Many complex flow phenomena have already been studied with this approach (see recent reviews [2, 3] and references therein). The LBE method is now an accurate engineering tool for simulating inert turbulence and is at an ideal stage for extension to chemically reacting turbulent flows.

We propose the development of a new methodology for calculating turbulent combustion based on the Boltzman equation rather than Navier-Stokes equation. Our ultimate objective is to perform large eddy simulations of the Lattice Boltzman equation (LBE-LES) for chemically reacting turbulent flows. The Boltzman equation is potentially a better hydrodynamic platform for LES calculations of turbulent combustion than is the Navier-Stokes equation. The advantages lay both in improved physical accuracy and better computational characteristics.

Computational advantages.

1. The LBE method solves a simplified version of the Boltzmann equation with a linear advection term and a local collision term. In NS methods, the advection term is non-linear and both the advection and viscous terms are non-local.

2. In the LBE method, the pressure is obtained *via* the simple ideal-gas equation of state, again a local calculation. In the continuum model, the pressure is typically obtained from a computationally intensive global solution of the Poisson equation.

3. Due to the locality of the numerical scheme, LBE is ideally suited for large-scale, especially, parallel computing. The scheme incurs very little communication penalty and in some special cases is known to scale superlinearly with increase in the number of processes. In principal, the LBE can also be solved with Boolean algorithms resulting in even faster computations [4].

4. Due to the kinetic nature of the LB method, it is particularly easy to handle complicated boundary geometries (including phase interfaces, flame fronts) without sacrificing computational speed. The treatment of complex boundaries in the NS-methods can get very tedious.

5. Multi-phase flow and flows with phase transitions can be easily handled in the LB method since all the hydrodynamic and thermodynamic properties are available locally. In the NS methods, calculating these features can be prohibitively expensive.

6. Multi-component diffusion can present a daunting computational challenge in NS methods. That can be handled with relative ease in the LB methods.

Physical advantages.

1. *LBE is more easily amenable to subgrid-scale modeling than is the Navier-Stokes equation.* This is due to the fact that the advection operator is linear.

2. The molecular-diffusion process which is a major source of modeling error in the PDF method appears in closed form in the LBE approach. In the PDF-method, a stochastic model is typically used for modeling this process.

3. With the LB-based methods, one has the choice of using a deterministic or a stochastic calculation for chemical kinetics. The stochastic method has several advantages over the deterministic scheme.

4. The LB-based models are better capable of accurately accounting for turbulence-chemistry interactions.

5. Advection (large-scale stirring) appears in closed form in both the methods.

2 LES of Boltzman equation for turbulent combustion.

Filtered Boltzman equation for turbulent reacting flows. We start with the one-particle velocity distribution function $f(\mathbf{v}; \mathbf{x}, t)$. According to the Boltzman equation, the distribution function of a species β evolves as:

$$\frac{\partial f_\beta}{\partial t} + v_j \frac{\partial f_\beta}{\partial x_j} = J_\beta = C_\beta + R_\beta. \tag{1}$$

The left hand side represents the advection of the distribution function in velocity phase space and J_β represents the collision operator for species β. If the flow is reacting, then the collision term can be split into two parts: one part due to non-reacting (inert) elastic collisions (C_β) and the second part due to reactive collisions (R_β). The distribution function f_β is normalized such that the species continuum density (ρ_β) and temperature (T_β) are obtained from the following integrations:

$$\rho_\beta(t) = \int m f_\beta(\mathbf{v}, t) d\mathbf{v}; \quad \frac{3}{2} \rho_\beta T_\beta(t) = \int (\frac{1}{2} m v^2) f_\beta(\mathbf{v}, t) d\mathbf{v}. \tag{2}$$

In the above m is the particle mass and κ is the Boltzman constant.

In the LES of the Navier-Stokes equations, the velocity and the scalar fields are decomposed into two parts: one part representing the resolved scales of motion and the second from the unresolved scales. Here, we perform a similar decomposition of the velocity distribution function.

$$f(\mathbf{v}, \mathbf{x}, t) = f^<(\mathbf{v}; \mathbf{x}, t) + f^>(\mathbf{v}; \mathbf{x}, t), \tag{3}$$

where, as per standard convention, the superscripts $<$ and $>$ represent, repspectively, the resolved and unresolved parts of the distribution function. We reiterate here that $\mathbf{v}$ is a phase-space variable and is absolutely unaffected by the filtering in physical space. From equation (1), we can write the evolution equations of the resolved and unresolved distribution functions:

$$\frac{\partial f_\beta^<}{\partial t} + v_j \frac{\partial f_\beta^<}{\partial x_j} = C_\beta^< + R_\beta^<; \quad \frac{\partial f_\beta^>}{\partial t} + v_j \frac{\partial f_\beta^>}{\partial x_j} = [C_\beta - C_\beta^<] + [R_\beta - R_\beta^<]. \tag{4}$$

The resolved distribution function deserves some discussion. Since advection process linear in the velocity distribution function, the left hand side of the above equation needs no closure modeling. Whereas, with the Navier-Stokes equation, filtering of the non-linear advection operator leads to unclosed terms which are the main sources of modeling error. In the filtered Boltzman equation, the non-linearity appears in a more benign algebraic form in the collision operator. The terms $C_\beta^<$ and $R_\beta^<$ certainly need closure modeling. It is expected that the modeling of these terms would be less challenging than their NS counterparts. One of the reasons is that the the resolved continuum variables (which is what we are after) are likely to be insensitive to the models of $C^<$ and $R^<$ at the mesoscopic scales. The closure modeling of these terms is the principle objective of the present research.

A second feature that make the LES of Boltzman equation very attractive for turbulent combustion is that fact that once the resolved distribution function is known, all the relevant resolved variables can be derived from it with no further approximation. Further, the relationship between the velocity distribution function and the continuum variables is linear in physical space:

$$\rho_\beta^< = \int m f_\beta^< d\mathbf{v}; \quad \rho_\beta^> = \int m f_\beta^> d\mathbf{v}; \quad (\rho_\beta \mathbf{u}_\beta)^< = \int m \mathbf{v} f_\beta^< d\mathbf{v}; \quad (\rho_\beta \mathbf{u}_\beta)^> = \int m \mathbf{v} f_\beta^> d\mathbf{v} \tag{5}$$

In the LES of the Navier-Stokes equations, subgrid-scale models are required for stresses, thermal flux and scalar flux. Further, models are also required for timescales of unresolved velocity, scalar and temperature fields. Models for these are typically derived independently based on different sets of assumptions. Even if each model is independently adequate, there is a real danger of incompatibility among them models resulting not only in large errors, but also in stifling numerical stiffness. In the LES of the Boltzman equation, all the models for all processes emerge from a single and, hence, internally-consistent methodology.

3 LBE-LES: Model development

Modeling of filtered non-reacting collision operator Non-reacting collisions in inert flows are typically modeled with the BGK approximation. The Boltzman equation with the BGK approximation is, in fact, the super-set of the Navier-Stokes equation. For a species β we have

$$C_\beta = -\omega_\beta(f_\beta - g_\beta); \quad C_\beta^< = -\omega_\beta(f_\beta^< - g_\beta^<), \tag{6}$$

where, ω_β is the inverse of the relaxation timescale and g_β is the Boltzman-Maxwell equilibrium distribution. *In the absence of reaction, the only term that is non-linear and, hence, needs closure modeling is the resolved-scale equilibrium distribution function.* The equilibrium distribution is of the form

$$g_\beta = \frac{\rho_\beta}{2\pi T_\beta} exp[-(\mathbf{v} - \mathbf{u})^2 / 2T_\beta]. \tag{7}$$

One of the main thrusts of the present research is to develop a closure model for $g^<$.

Modeling of reacting collision operator The reaction operator can be represented in several different ways depending on the degree of accuracy required. At the most fundamental level we can consider the reactions at the molecular collision level following the methodology of Kugerl (Solution of the Boltzman Equation for a reacting gas mixture, *Phil. Trans. R. Soc. Lond. A, 1993, pp 414 - 437*). Howvever, for most practical combustion applications the deterministic reaction-rate approach will be quite adequate. For the Lattice-Boltzman equation method we will use the standard deterministic law of mass-action, Arrhenius-type reaction model. The modeling and numerical issues will then be similar to t'·ose encountered on Navier-Stokes hydrodynamic platforms and similar strategies can be used. If, however, one were to use the Lattice Gas Automata scheme, stochastic approaches are possible for computing reactions. This stochastic chemistry method is definitely superior to the deterministic method both in terms of theoretical validity and computability. These issues will be addressed in detail in the present research.

Reduced-chemistry models. If the deterministic chemistry approach is used, ways must be found to obtain reduced representations for the full chemical kinetics. Some of the simpler methods (quasi-steady state approximation and partial equilibrium approximation) tend to be too inaccurate and the more sophisticated ones (ILDM. CSP) continue to be too computation intensive. Two procedures that are adequately accurate and computationally viable are the minimization of the evolution rate method [5] and a high-order quasi-steady state approximation currently under development [6].

Conclusion We propose the development of an innovative computational tool for turbulent combustion that is based on the Boltzman equation rather than on the navier-Stokes equation. The proposed LBE-LES method for turbulent combustion is still very much in its infancy, offering a tremendous opportunity for ground-breaking advancement.

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